

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052815\
 Data File : BG017349.D
 Acq On : 29 May 2015 7:37
 Operator : TP/IZ
 Sample : G2386-23
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-13-SS

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.762	349	353	362	rVB	29182	41817	3.04%	0.425%
2	5.249	430	436	449	rBV	258199	368456	26.83%	3.743%
3	6.853	703	709	717	rBV	306427	480128	34.96%	4.877%
4	7.194	759	767	776	rBV	322520	494445	36.00%	5.022%
5	7.652	839	845	852	rVB2	111332	165311	12.04%	1.679%
6	7.976	890	900	909	rBV	303710	483865	35.23%	4.915%
7	8.816	1035	1043	1051	rBV	269638	440282	32.06%	4.472%
8	10.443	1314	1320	1327	rBV	136911	235442	17.14%	2.392%
9	12.929	1735	1743	1756	rBV	636507	902253	65.69%	9.165%
10	13.775	1882	1887	1894	rBV	34478	47736	3.48%	0.485%
11	14.309	1972	1978	1987	rBV2	207208	348981	25.41%	3.545%
12	15.802	2227	2232	2243	rVB2	393653	595873	43.38%	6.053%
13	17.059	2440	2446	2450	rBV	294034	400079	29.13%	4.064%
14	17.100	2450	2453	2460	rVB	85547	103813	7.56%	1.055%
15	17.194	2465	2469	2474	rVB	16760	23931	1.74%	0.243%
16	17.464	2508	2515	2519	rBV3	9414	14948	1.09%	0.152%
17	17.964	2592	2600	2609	rBV6	34391	64646	4.71%	0.657%
18	18.134	2622	2629	2632	rBV2	16686	28220	2.05%	0.287%
19	19.121	2792	2797	2807	rVB	187580	233372	16.99%	2.371%
20	19.486	2849	2859	2868	rBV	154599	241261	17.57%	2.451%
21	19.697	2884	2895	2900	rBV	1132278	1373517	100.00%	13.952%
22	19.985	2934	2944	2947	rBV	26177	50849	3.70%	0.517%
23	20.085	2958	2961	2964	rVB	23369	25331	1.84%	0.257%
24	20.144	2964	2971	2975	rBV5	10564	24755	1.80%	0.251%
25	20.896	3095	3099	3103	rBV3	11522	16570	1.21%	0.168%
26	20.960	3106	3110	3117	rVB3	97300	135775	9.89%	1.379%
27	21.248	3149	3159	3163	rBV2	441400	681478	49.62%	6.922%
28	21.283	3163	3165	3171	rVB	91496	99772	7.26%	1.013%
29	21.401	3181	3185	3189	rBV3	25070	32689	2.38%	0.332%
30	21.789	3246	3251	3255	rBV5	14573	22878	1.67%	0.232%
31	21.842	3255	3260	3264	rBV6	17579	33863	2.47%	0.344%
32	22.024	3289	3291	3297	rVB6	15494	21686	1.58%	0.220%
33	22.088	3298	3302	3307	rVB8	11202	19769	1.44%	0.201%
34	22.282	3331	3335	3340	rBV7	10677	21605	1.57%	0.219%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	22.417	3354	3358	3362	rBV6	14658	20527	1.49%	0.209%
36	22.811	3419	3425	3430	rBV2	96527	229540	16.71%	2.332%
37	22.981	3450	3454	3459	rVB3	22544	39031	2.84%	0.396%
38	23.293	3502	3507	3514	rVB	50480	96738	7.04%	0.983%
39	23.387	3517	3523	3532	rVB	74165	139307	10.14%	1.415%
40	23.487	3533	3540	3546	rBV	253320	489416	35.63%	4.971%
41	24.021	3629	3631	3637	rVB6	20786	30017	2.19%	0.305%
42	25.766	3923	3928	3934	rVB2	35731	82591	6.01%	0.839%
43	26.466	4041	4047	4056	rBV2	26970	77898	5.67%	0.791%
44	26.836	4102	4110	4119	rVB10	62864	183782	13.38%	1.867%
45	27.741	4255	4264	4276	rVB10	39267	156654	11.41%	1.591%
46	28.687	4419	4425	4426	rBV6	14595	23768	1.73%	0.241%

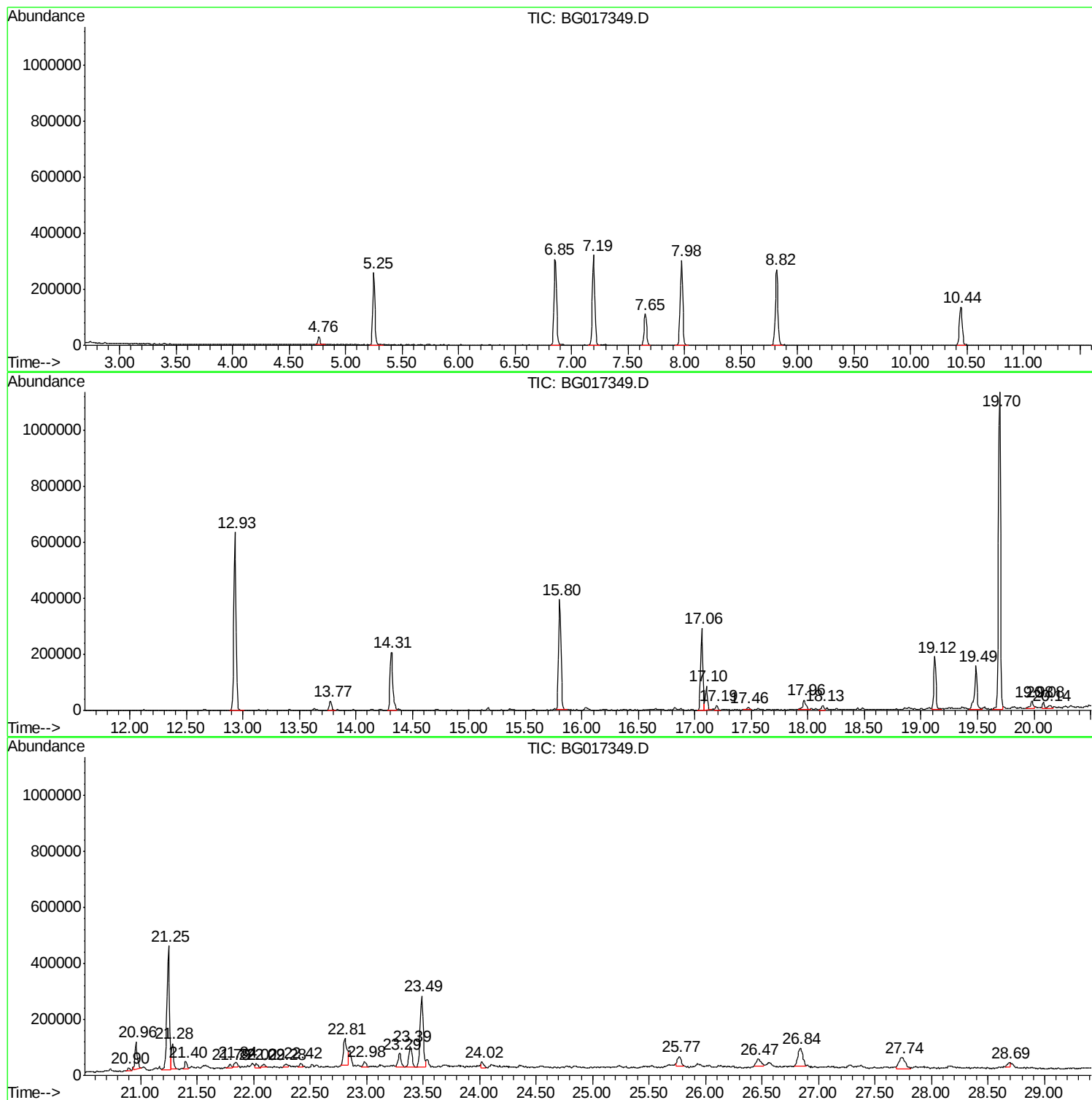
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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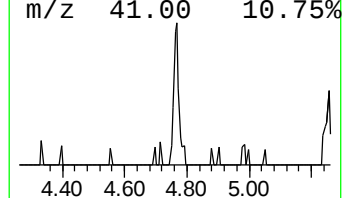
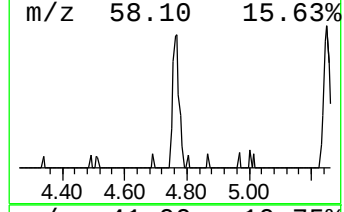
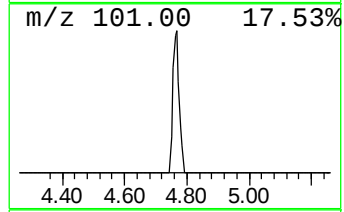
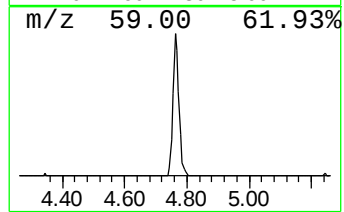
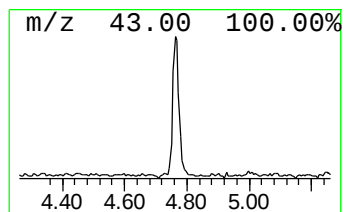
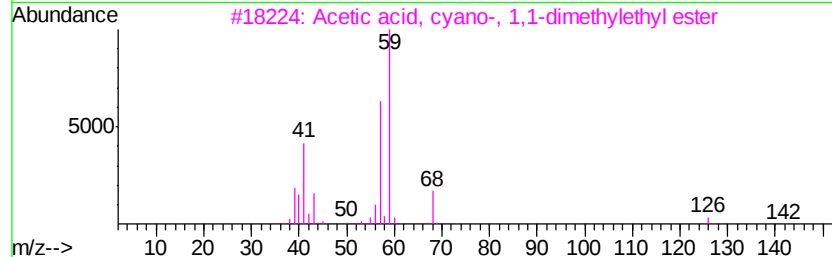
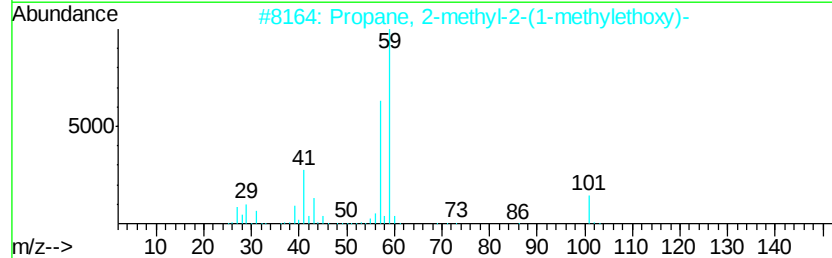
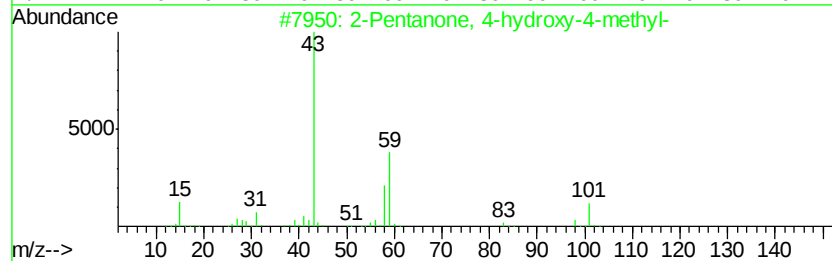
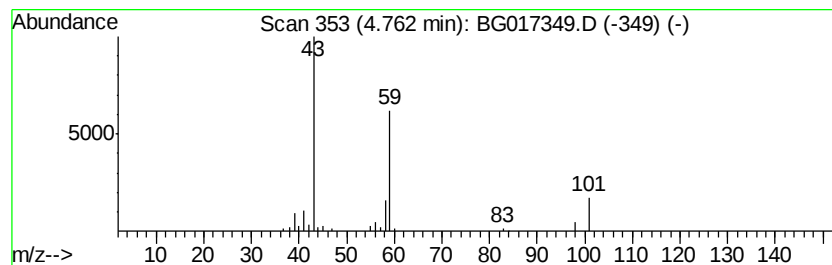
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	5.06 ng	41817	1,4-Dichlorobenzene-d4	7.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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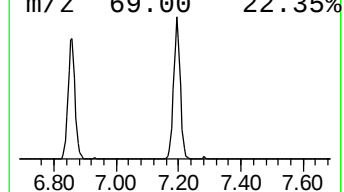
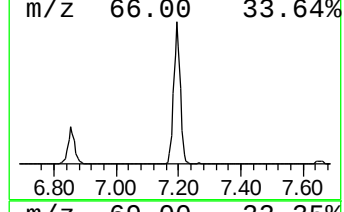
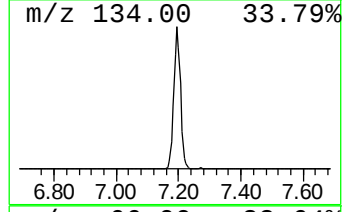
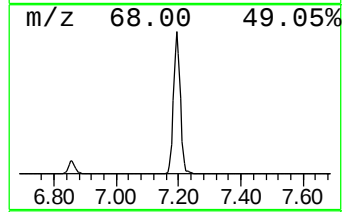
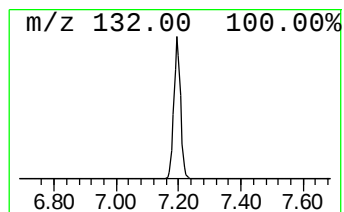
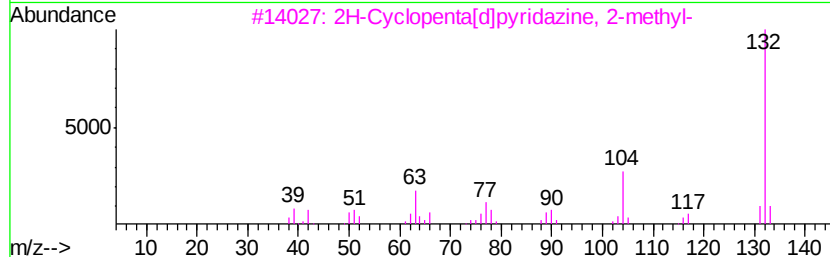
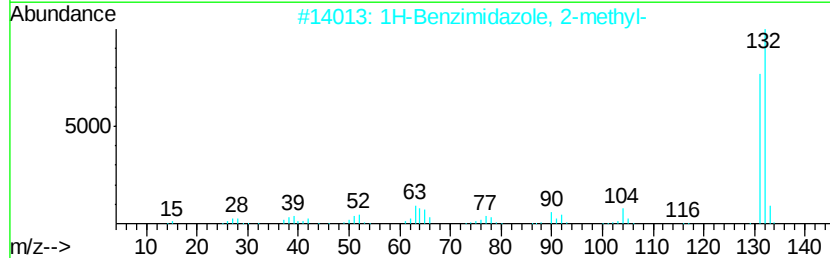
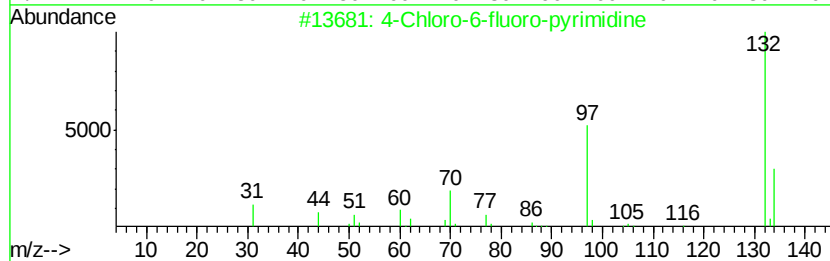
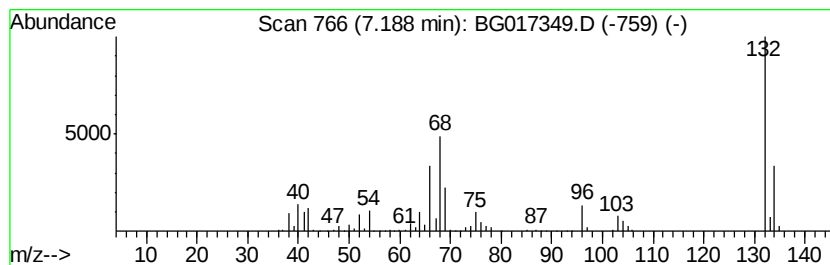
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	59.82 ng	494445	1,4-Dichlorobenzene-d4	7.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5			Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	12



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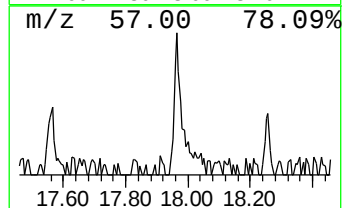
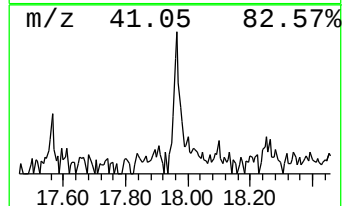
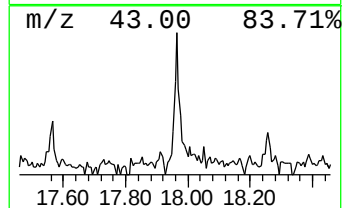
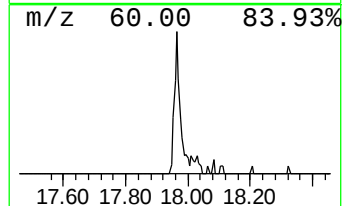
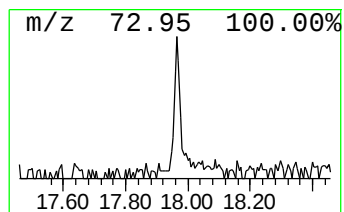
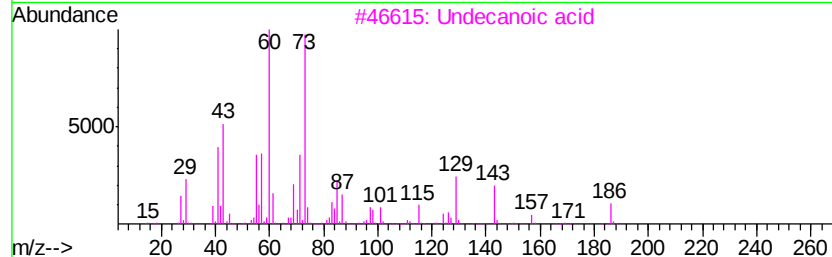
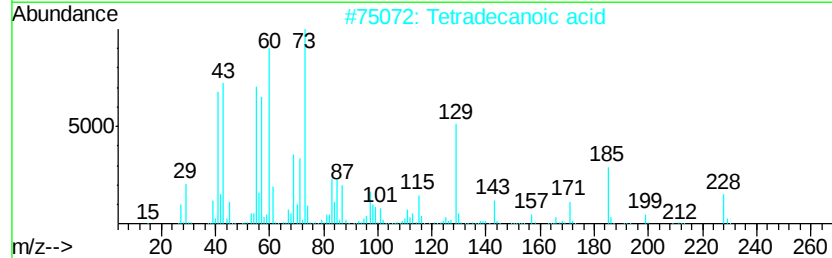
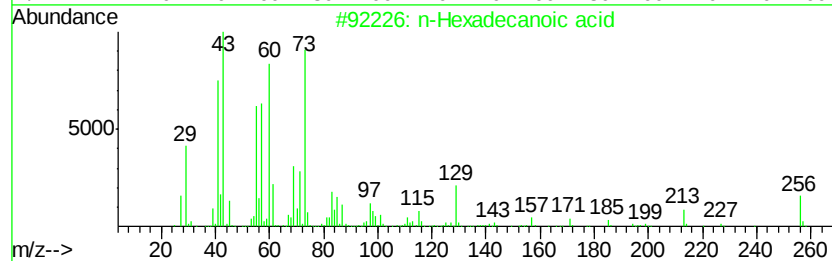
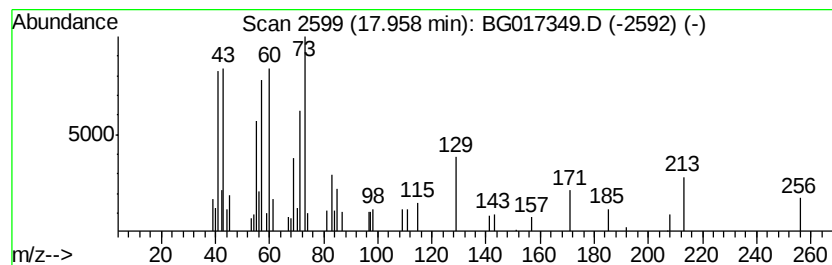
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	3.23 ng	64646	Phenanthrene-d10	17.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Undecanoic acid	186	C11H22O2	000112-37-8	53
4		n-Decanoic acid	172	C10H20O2	000334-48-5	52
5		Tridecanoic acid	214	C13H26O2	000638-53-9	50



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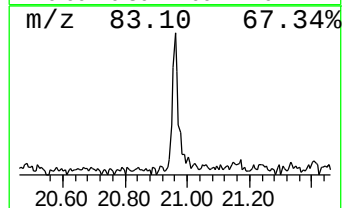
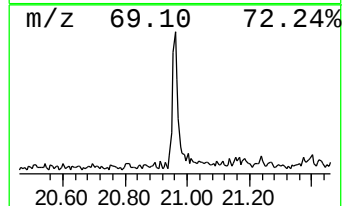
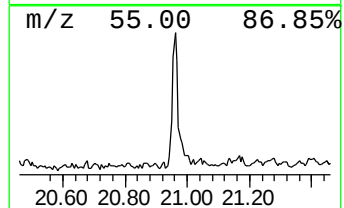
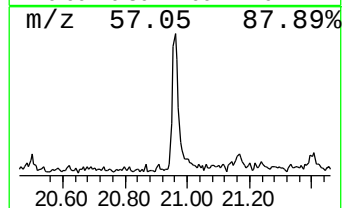
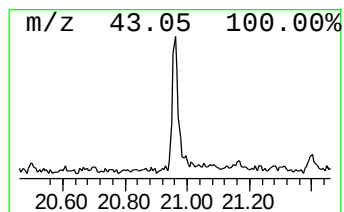
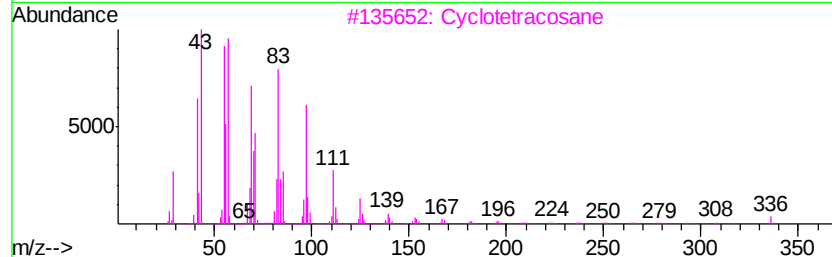
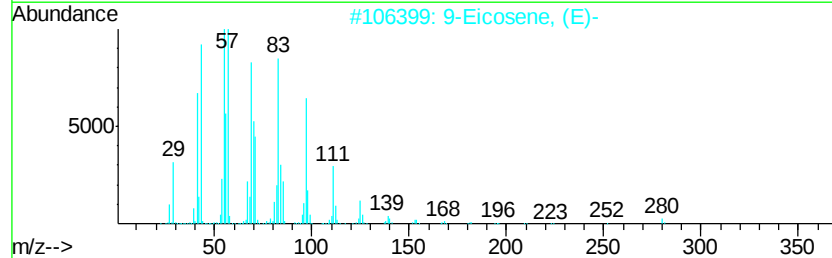
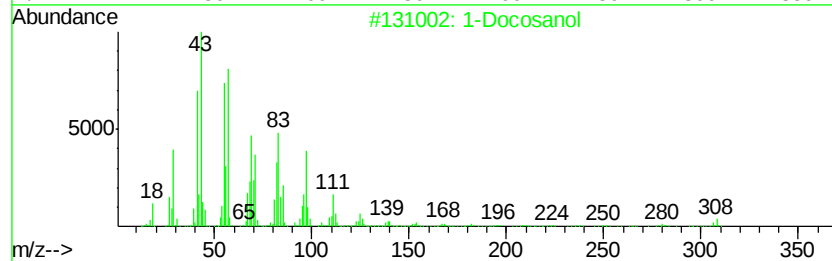
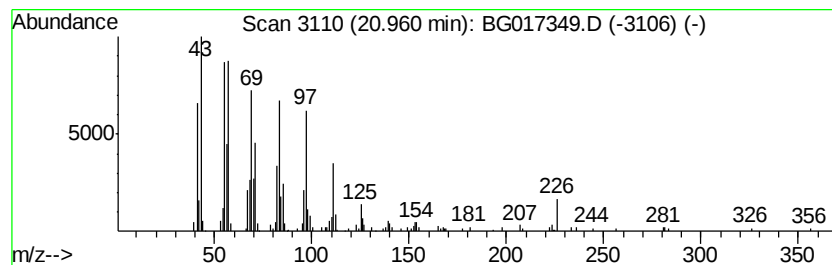
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.96	3.98 ng	135775	Chrysene-d12	21.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanol	326	C22H46O	000661-19-8	90
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
3	Cyclotetracosane	336	C24H48	000297-03-0	90
4	Cycloeicosane	280	C20H40	000296-56-0	89
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87



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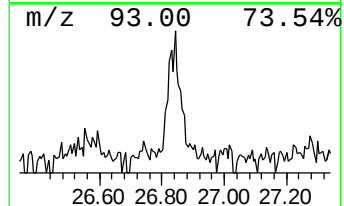
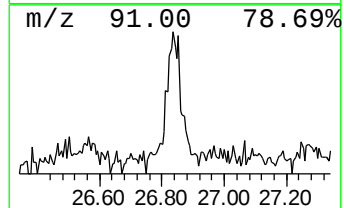
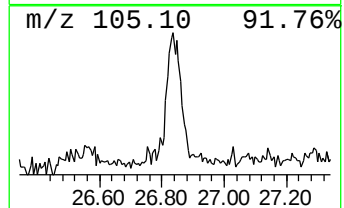
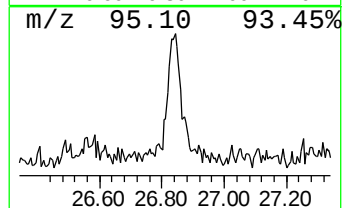
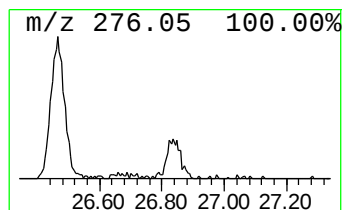
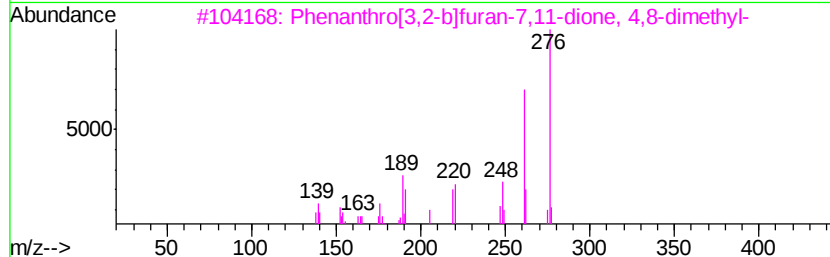
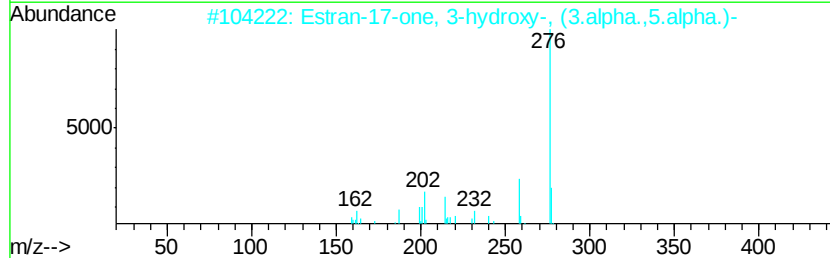
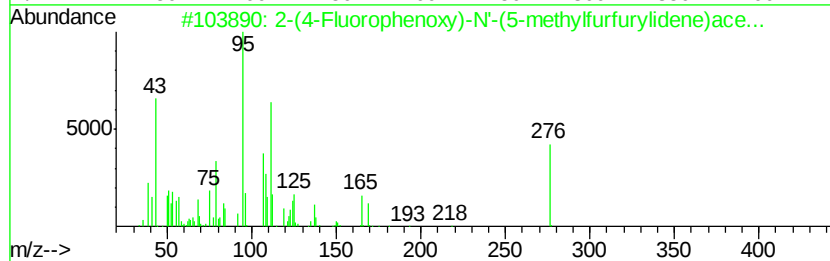
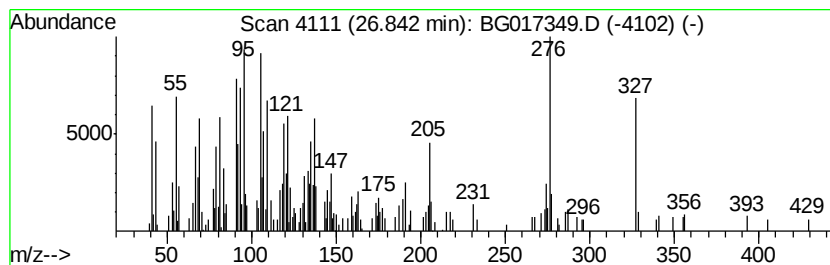
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown26.84 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.84	7.51 ng	183782	Perylene-d12	23.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(4-Fluorophenoxy)-N'-(5-methyl...	276	C14H13FN2O3	339121-32-3	30
2		Estran-17-one, 3-hydroxy-, (3.alpha...	276	C18H28O2	001225-01-0	25
3		Phenanthro[3,2-b]furan-7,11-dion...	276	C18H12O3	020958-17-2	25
4		Longifolenaldehyde	220	C15H24O	019890-84-7	16
5		9,19-Cyclolanost-24-en-3-ol, ace...	468	C32H52O2	001259-10-5	16



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052815\
Data File : BG017349.D
Acq On : 29 May 2015 7:37
Operator : TP/IZ
Sample : G2386-23
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13-SS

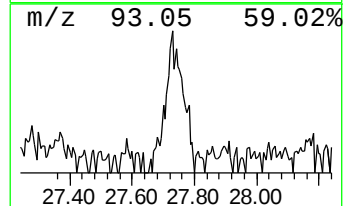
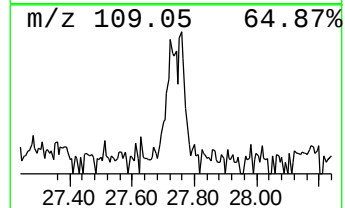
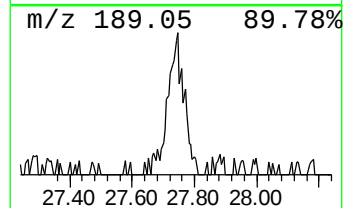
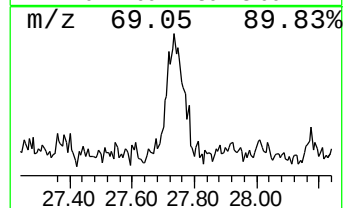
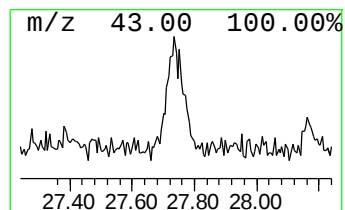
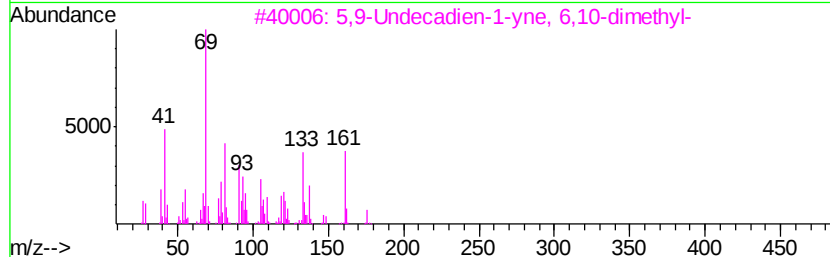
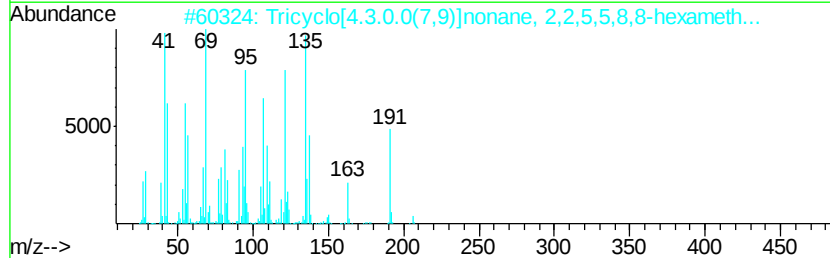
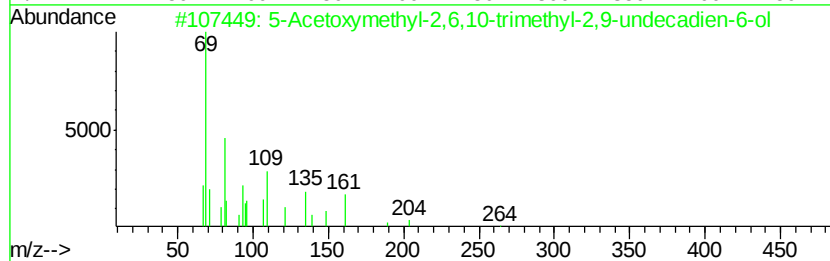
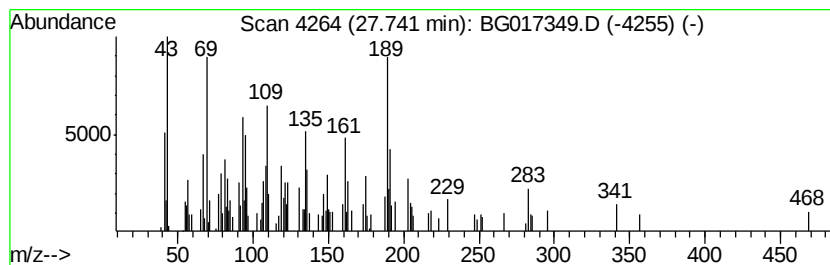
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown27.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.74	6.40 ng	156654	Perylene-d12	23.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Acetoxymethyl-2,6,10-trimethyl...	282	C17H30O3	1000144-12-3	32
2		Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	32
3		5,9-Undecadien-1-yne, 6,10-dimet...	176	C13H20	100451-98-7	25
4		Silane, triethyl(2-phenylethenyl)-	218	C14H22Si	001206-29-7	18
5		p-Menthon-8-thiol	186	C10H18OS	033281-91-3	14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052815\
Data File : BG017349.D
Acq On : 29 May 2015 7:37
Operator : TP/IZ
Sample : G2386-23
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13-SS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	5.1	ng	41817	1	7.65	165311	20.0
unknown7.19	7.19	59.8	ng	494445	1	7.65	165311	20.0
n-Hexadecanoic acid	17.96	3.2	ng	64646	4	17.06	400079	20.0
1-Docosanol	20.96	4.0	ng	135775	5	21.25	681478	20.0
unknown26.84	26.84	7.5	ng	183782	6	23.49	489416	20.0
unknown27.74	27.74	6.4	ng	156654	6	23.49	489416	20.0